Supplementary Information

New Synthetic Quinolines as Cathepsin K Inhibitors

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General information

The niobium pentachloride (NbCl₅) was supplied by Companhia Brasileira de Metalurgia e Mineração (CBMM, Araxá, Minas Gerais, Brazil) and used as received. All the other reagents were purchased from Merck (Kenilworth, New Jersey, USA). When necessary, solvents and reagents were purified and dried before use by routine methods. ¹H, ¹³C and DEPT-135 NMR spectra were recorded with a Bruker DRX-400 AVANCE spectrometer at 400.15, 100.62 and 100.62 MHz, respectively, using CDCl₃ (or DMSO-d₆) as solvent and tetramethylsilane (TMS) as internal reference standard. The chemical shifts are expressed in δ (ppm) and the coupling constants (J) in hertz (Hz). Gravity column chromatography was performed on silica gel (70-230 mesh, 63-200 μM, pore size 60 Å) purchased from Merck (Kenilworth, New Jersey, USA). Analytical thin-layer chromatography (TLC) was performed on Merck aluminum sheets coated with silica gel 60-F₂₅₄ and visualized with ultraviolet light (254 or 366 nm) or heating with TLC stains. FTIR spectra were recorded on a Shimadzu IR PRESTIGE-21 spectrophotometer using KBr pellets in the range of 4000-400 cm⁻¹. HRMS analyses were recorded on a Bruker micrOTOF-Q II mass spectrometer equipped with electron spray ionization-time of flight (ESI-TOF), operating in positive mode. The melting point was obtained from MQAPF-302 melting point apparatus (Microquímica® Equipamentos LTDA, Brazil). The organic solvents were evaporated using a Büchi Rotavapor R-215 at 40 °C.

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\(^1\)H, \(^1^3\)C and DEPT NMR and HRMS spectra of compounds 4a and 4g-4i

**Figure S1.** \(^1\)H NMR spectrum (400 MHz, CDCl\(_3\)) of compound 4a.
Figure S2. $^{13}$C NMR spectrum (100 MHz, CDCl$_3$) of compound 4a.
Figure S3. $^{13}$C DEPT-135 NMR spectrum (100 MHz, CDCl$_3$) of compound 4a.
Figure S4. Mass spectrum (HRMS-ESI-TOF) of compound 4a.

Calcd for C_{21}H_{16}N [M + H]^+ = 282.1277

Found for C_{21}H_{16}N [M + H]^+ = 282.1291
Figure S5. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 4g.
Figure S6. $^{13}$C NMR spectrum (100 MHz, CDCl$_3$) of compound 4g.
Figure S7. $^{13}$C DEPT-135 NMR spectrum (100 MHz, CDCl$_3$) of compound $4g$. 
Figure S8. Mass spectrum (HRMS-ESI-TOF) of compound 4g.

Calcd for C_{22}H_{13}N_2 [M + H]^+ = 307.1230

Found for C_{22}H_{13}N_2 [M + H]^+ = 307.1232
Figure S9. $^1$H NMR spectrum (400 MHz, CDCl$_3$) of compound 4h.
Figure S10. $^{13}$C NMR spectrum (100 MHz, CDCl$_3$) of compound 4h.
Figure S11. $^{13}$C DEPT-135 NMR spectrum (100 MHz, CDCl$_3$) of compound 4h.
**Figure S12.** Mass spectrum (HRMS-ESI-TOF) of compound 4h.
Figure S13. $^1$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 4i.
Figure S14. $^{13}$C NMR spectrum (100 MHz, DMSO-$d_6$) of compound 4i.
Figure S15. $^{13}$C DEPT-135 NMR spectrum (100 MHz, DMSO-$d_6$) of compound 4i.
**Figure S16.** Mass spectrum (HRMS-ESI-TOF) of compound 4i.